* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	Jun 03	New e-mail delivery for search results now available
NEWS 4	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 5	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 6	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 7	Sep 03	JAPIO has been reloaded and enhanced
NEWS 8	Sep 16	Experimental properties added to the REGISTRY file
NEWS 9	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 10	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 11	Oct 24	BEILSTEIN adds new search fields
NEWS 12	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 13	Nov 18	DKILIT has been renamed APOLLIT
NEWS 14	Nov 25	More calculated properties added to REGISTRY
NEWS 15	Dec 04	CSA files on STN .
NEWS 16	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 17	Dec 17	TOXCENTER enhanced with additional content
NEWS 18	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 19	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 20	Feb 13	CANCERLIT is no longer being updated
NEWS 21	Feb 24	METADEX enhancements
NEWS 22	Feb 24	PCTGEN now available on STN
NEWS 23	Feb 24	TEMA now available on STN
NEWS 24	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS 25	Feb 26	PCTFULL now contains images
NEWS 26	Mar 04	SDI PACKAGE for monthly delivery of multifile SDI results
NEWS 27	Mar 20	EVENTLINE will be removed from STN
NEWS 28	Mar 24	PATDPAFULL now available on STN
NEWS 29	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS 30	Apr 11	Display formats in DGENE enhanced
NEWS 31	Apr 14	MEDLINE Reload
NEWS 32	Apr 17	Polymer searching in REGISTRY enhanced
NEWS 33	Jun 13	Indexing from 1947 to 1956 added to records in CA/CAPLUS
NEWS 34	Apr 21	New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS 35	Apr 28	RDISCLOSURE now available on STN
NEWS 36	May 05	Pharmacokinetic information and systematic chemical names added to PHAR
NEWS 37	May 15	MEDLINE file segment of TOXCENTER reloaded
NEWS 38	May 15	Supporter information for ENCOMPPAT and ENCOMPLIT updated
NEWS 39	May 16	CHEMREACT will be removed from STN
NEWS 40	May 19	Simultaneous left and right truncation added to WSCA
NEWS 41	May 19	RAPRA enhanced with new search field, simultaneous left and right truncation
NEWS 42	Jun 06	Simultaneous left and right truncation added to CBNB
NEWS 43	Jun 06	PASCAL enhanced with additional data
NEWS 44	Jun 20	2003 edition of the FSTA Thesaurus is now available
NEWS 45	Jun 25	HSDB has been reloaded

NEWS EXPRESS	April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items

NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 05:20:39 ON 30 JUN 2003

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 05:20:47 ON 30 JUN 2003
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STRUCTURE FILE UPDATES: 27 JUN 2003 HIGHEST RN 539020-41-2
DICTIONARY FILE UPDATES: 27 JUN 2003 HIGHEST RN 539020-41-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

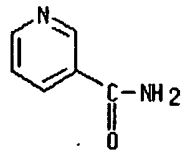
=> e nicotinamide/cn
E1 1 NICOTINAMIDASE/ PYRAZINAMIDASE (SALMONELLA ENTERICA TYPHIMURIUM STRAIN LT2; SGSC 1412; ATCC 700720 GENE PNCA)/CN
E2 1 NICOTINAMIDASE/PYRAZINAMIDASE (PSEUDOMONAS STRAIN ADP GENE ATZE)/CN
E3 1 --> NICOTINAMIDE/CN
E4 1 NICOTINAMIDE (5-(BROMOACETYL)-4-METHYLIMIDAZOLE) DINUCLEOTIDE/CN
E5 1 NICOTINAMIDE 1,N6-ETHENOADENINE DINUCLEOTIDE/CN
E6 1 NICOTINAMIDE 1,N6-ETHENOADENINE DINUCLEOTIDE PHOSPHATE/CN
E7 1 NICOTINAMIDE 2'-DEOXYADENOSINE DINUCLEOTIDE/CN
E8 1 NICOTINAMIDE 2'-DEOXYADENOSINE DINUCLEOTIDE, REDUCED/CN
E9 1 NICOTINAMIDE 2-AMINO-4-(METHOXYMETHYL)-6-METHYL-/CN
E10 1 NICOTINAMIDE 2-AMINOPURINE RIBOSIDE DINUCLEOTIDE/CN
E11 1 NICOTINAMIDE 3,N4-ETHENOCYTOSINE DINUCLEOTIDE/CN
E12 1 NICOTINAMIDE 3-DEAZAPURINE DINUCLEOTIDE/CN

```
=> s e3
L1            1 NICOTINAMIDE/CN

=> d l1

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2003 ACS
RN   98-92-0  REGISTRY
CN   3-Pyridinecarboxamide (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Nicotinamide (8CI)
OTHER NAMES:
CN   β-Pyridinecarboxamide
CN   3-(Aminocarbonyl)pyridine
CN   3-Amidopyridine
CN   3-Carbamoylpyridine
CN   3-Pyridinecarboxylic acid amide
CN   Aminicotin
CN   Benicot
CN   Delonin Amide
CN   Dipegyl
CN   m-(Aminocarbonyl)pyridine
CN   NAM
CN   Niacinamide
CN   Niavit PP
CN   Nicamina
CN   Nicamindon
CN   Nicasir
CN   Nicobion
CN   Nicofort
CN   Nicosan 2
CN   Nicosylamide
CN   Nicotilamide
CN   Nicotine acid amide
CN   Nicotinic acid amide
CN   Nicotinic amide
CN   Nicotylamide
CN   Nicovit
CN   Nicovitina
CN   Nictoamide
CN   Niocinamide
CN   Niozymin
CN   Papulex
CN   Pelmin
CN   Pelmine
CN   Pelonin amide
CN   Vi-Nicotyl
CN   Vitamin B
CN   Vitamin B3
FS   3D CONCORD
DR   123574-63-0, 37321-14-5, 78731-47-2
MF   C6 H6 N2 O
CI   COM
LC   STN Files:   ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*,
       BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS,
       CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM,
       CSNB, DDFU, DETHERM*, DIOGENES, DRUGU, EMBASE, GMELIN*, HODOC*, HSDB*,
       IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT,
       NIOSHTIC, PDLCOM*, PHAR, PIRA, PROMT, RTECS*, SPECINFO, TOXCENTER, USAN,
       USPAT2, USPATFULL, VTB
```

(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7618 REFERENCES IN FILE CA (1957 TO DATE)
267 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
7620 REFERENCES IN FILE CAPLUS (1957 TO DATE)
9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
=> e cyanopyridine/cn
E1            1     CYANOPTERINE/CN
E2            1     CYANOPYRAZINE/CN
E3            1 --> CYANOPYRIDINE/CN
E4            1     CYANOPYRIDINIUM BROMIDE/CN
E5            1     CYANOQUINONAMINE/CN
E6            1     CYANORESIN CR-C/CN
E7            1     CYANORESIN CR-E/CN
E8            1     CYANORESIN CR-E TRIFLUOROMETHYLBENZOATE/CN
E9            1     CYANORESIN CR-M/CN
E10           1     CYANORESIN CR-S/CN
E11           1     CYANORESIN CR-S BENZOATE/CN
E12           1     CYANORESIN CR-S FLUOROBENZOATE/CN

=> s e3
L2            1 CYANOPYRIDINE/CN

=> d 12

L2   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2003 ACS
RN   29386-66-1  REGISTRY
CN   Pyridinecarbonitrile (6CI, 8CI, 9CI)  (CA INDEX NAME)
OTHER NAMES:
CN   Cyanopyridine
MF   C6 H4 N2
CI   IDS
LC   STN Files:   BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CIN, PROMT,
       TOXCENTER, USPAT2, USPATFULL
```

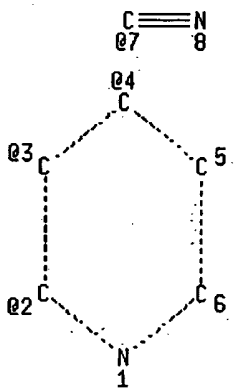
D1-CN

65 REFERENCES IN FILE CA (1957 TO DATE)
6 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
65 REFERENCES IN FILE CAPLUS (1957 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=>
L3 STRUCTURE UPLOADED

=> d 13
L3 HAS NO ANSWERS
L3 STR



VPA 7-2/3/4 S
NODE ATTRIBUTES:
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
NSPEC IS R AT 4
NSPEC IS R AT 5
NSPEC IS R AT 6
NSPEC IS C AT 7
NSPEC IS C AT 8
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 7 8
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

=> s l3
SAMPLE SEARCH INITIATED 05:24:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5903 TO ITERATE

16.9% PROCESSED 1000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 113456 TO 122664
PROJECTED ANSWERS: 32894 TO 37942

L4 50 SEA SSS SAM L3

=> s l3 full

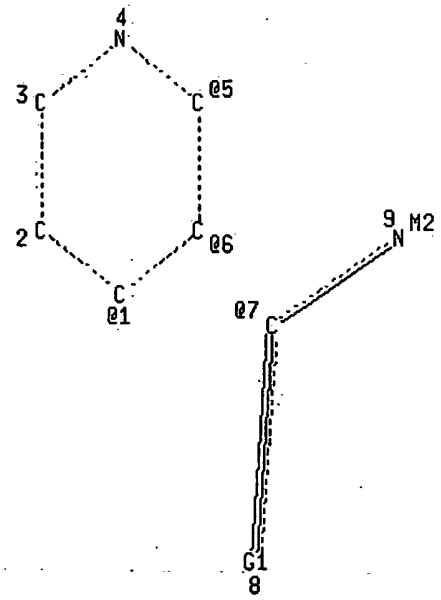
```
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 05:25:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 118278 TO ITERATE

100.0% PROCESSED  118278 ITERATIONS                    34801 ANSWERS
SEARCH TIME: 00.00.01

L5        34801 SEA SSS FUL L3

=>
L6      STRUCTURE UPLOADED

=> d 16
L6 HAS NO ANSWERS
L6                STR
 0 10 S 11
Page 1-A
```




```
Page 1-B
VAR G1=10/11
VPA 7-1/5/6 S
NODE ATTRIBUTES:
HCOUNT   IS M2      AT   9
NSPEC    IS R       AT   1
NSPEC    IS R       AT   2
NSPEC    IS R       AT   3
NSPEC    IS R       AT   4
NSPEC    IS R       AT   5
NSPEC    IS R       AT   6
NSPEC    IS C       AT   7
NSPEC    IS C       AT   8
NSPEC    IS C       AT   9
DEFAULT MLEVEL IS ATOM
MLEVEL   IS CLASS   AT   7  9 10 11
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  11
```

```
STEREO ATTRIBUTES: NONE


=> s l6
SAMPLE SEARCH INITIATED 05:26:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  27967 TO ITERATE

  3.6% PROCESSED    1000 ITERATIONS                              18 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       549361 TO   569319
PROJECTED ANSWERS:            8722 TO    11414

L7           18 SEA SSS SAM L6

=> file hcaplus
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                163.95     164.16

FILE 'HCAPLUS' ENTERED AT 05:27:14 ON 30 JUN 2003
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FILE COVERS 1907 - 30 Jun 2003  VOL 139 ISS 1
FILE LAST UPDATED: 29 Jun 2003  (20030629/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> d his

     (FILE 'HOME' ENTERED AT 05:20:39 ON 30 JUN 2003)

     FILE 'REGISTRY' ENTERED AT 05:20:47 ON 30 JUN 2003
                E NICOTINAMIDE/CN
L1            1 S E3
                E CYANOPYRIDINE/CN
L2            1 S E3
L3              STRUCTURE UPLOADED
L4           50 S L3
L5        34801 S L3 FULL
L6              STRUCTURE UPLOADED
```

```
L7            18 S L6

     FILE 'HCAPLUS' ENTERED AT 05:27:14 ON 30 JUN 2003

=> s l1/prep
          7664 L1
       3020723 PREP/RL
L8          250 L1/PREP
                (L1 (L) PREP/RL)

=> s l5/rct
         10933 L5
       2532391 RCT/RL
L9          5151 L5/RCT
                (L5 (L) RCT/RL)

=> s l9 and l8
L10           80 L9 AND L8

=> file reg
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                               4.51     168.67

FILE 'REGISTRY' ENTERED AT 05:28:15 ON 30 JUN 2003
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STRUCTURE FILE UPDATES:  27 JUN 2003  HIGHEST RN 539020-41-2
DICTIONARY FILE UPDATES:  27 JUN 2003  HIGHEST RN 539020-41-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> e water/cn
E1            1     WATCON 1255/CN
E2            1     WATCON 130/CN
E3            1 --> WATER/CN
E4            1     WATER ((H2O)2)/CN
E5            1     WATER (D2180)/CN
E6            1     WATER (D2O1+)/CN
E7            1     WATER (DOT), HEAVY/CN
E8            1     WATER (DTO)/CN
E9            1     WATER (H17OH)/CN
E10           1     WATER (H2140)/CN
E11           1     WATER (H2150)/CN
E12           1     WATER (H2170)/CN
```

```
=> s e3
L11           1 WATER/CN

=> d l11

L11  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2003 ACS
RN   7732-18-5  REGISTRY
CN   Water (8CI, 9CI)  (CA INDEX NAME)
OTHER NAMES:
CN   1593: PN: WO03025132 TABLE: 42 claimed sequence
CN   Distilled water
CN   DRiWATER
CN   Hydrogen oxide (H2O)
CN   R 718
FS   3D CONCORD
MF   H2 O
CI   COM
LC   STN Files:   ANABSTR, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAPLUS,
       CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CSCHEM,
       CSNB, DETHERM*, DIPPR*, EMBASE, GMELIN*, IFICDB, IFIPAT, IFIUDB, IPA,
       MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, RTECS*, SPECINFO,
       TOXCENTER, ULIDAT, USAN, USPAT2, USPATFULL, VTB
         (*File contains numerically searchable property data)
     Other Sources:   DSL**, EINECS**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)


 H2O

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

          287130 REFERENCES IN FILE CA (1957 TO DATE)
             955 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
          287291 REFERENCES IN FILE CAPLUS (1957 TO DATE)


=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     6.30     174.97

FILE 'HCAPLUS' ENTERED AT 05:28:39 ON 30 JUN 2003
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FILE COVERS 1907 - 30 Jun 2003  VOL 139 ISS 1
```

```
FILE LAST UPDATED: 29 Jun 2003  (20030629/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> d his

     (FILE 'HOME' ENTERED AT 05:20:39 ON 30 JUN 2003)

     FILE 'REGISTRY' ENTERED AT 05:20:47 ON 30 JUN 2003
                E NICOTINAMIDE/CN
L1            1 S E3
                E CYANOPYRIDINE/CN
L2            1 S E3
L3              STRUCTURE UPLOADED
L4           50 S L3
L5        34801 S L3 FULL
L6              STRUCTURE UPLOADED
L7           18 S L6

     FILE 'HCAPLUS' ENTERED AT 05:27:14 ON 30 JUN 2003
L8          250 S L1/PREP
L9         5151 S L5/RCT
L10          80 S L9 AND L8

     FILE 'REGISTRY' ENTERED AT 05:28:15 ON 30 JUN 2003
                E WATER/CN
L11           1 S E3

     FILE 'HCAPLUS' ENTERED AT 05:28:39 ON 30 JUN 2003

=> s l11/rct
        287548 L11
       2532391 RCT/RL
L12      21445 L11/RCT
                (L11 (L) RCT/RL)

=> s l12 and l10
L13           0 L12 AND L10

=> s l10 and metal?
       2062308 METAL?
L14           7 L10 AND METAL?

=> s l14 and catal?
       1182962 CATAL?
L15           5 L14 AND CATAL?

=> d l15, ibib abs hitstr, 1-5

L15  ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2003 ACS
```

Full Text | Citing References

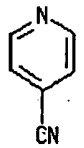
```
ACCESSION NUMBER:          2003:98167  HCAPLUS
DOCUMENT NUMBER:           138:287778
TITLE:                     Organometallic Chemistry in Aqueous Solution.
                           Hydration of Nitriles to Amides Catalyzed by a
                           Water-Soluble Molybdocene, (MeCp)2Mo(OH)(H2O)+
AUTHOR(S):                 Breno, Kerry L.; Pluth, Michael D.; Tyler, David R.
```

CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene, OR, 97403, USA
SOURCE: Organometallics (2003), 22(6), 1203-1211
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

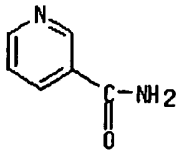
AB [Cp'2Mo(μ-OH)2MoCp'2]2+ (1) (Cp' = η5-CH3C5H4) is a precatalyst for the hydration of nitriles in aq. soln. under mild conditions (~80°). Among the nitriles hydrated were acetonitrile, isobutyronitrile, benzonitrile, 3-hydroxypropionitrile, 3-bromopropioamide, 4-cyanopyridine, succinonitrile, Me cyanoacetate, 2-methoxyacetonitrile, and acrylonitrile. Except in the case of 2-methoxyacetonitrile, hydrolysis of the resulting amide products did not occur. Hydration of the C:C double bond did not occur in acrylonitrile, but hydrolysis of ester and ether linkages did occur in nitriles contg. those functional groups. The apparent rate consts. and turnover frequencies of the **catalytic** reactions were detd. using an iterative kinetics-fitting program. The rates and turnover frequencies are comparable to those reported for many homogeneous nitrile hydration **catalysts** described in the literature. In aq. soln., 1 is in equil. with [Cp'2Mo(OH)(H2O)]+ (2), and this monomer is proposed to be the active hydration **catalyst**. The hydration is proposed to occur by an intramol. attack of a hydroxide ligand on a coordinated nitrile. The hydration reaction is irreversibly inhibited by product and reversibly inhibited by substrate (nitrile).

IT 100-48-1, 4-Cyanopyridine
RL: PRP (Properties); **RCT (Reactant)**; RACT (Reactant or reagent)
(hydration kinetics; kinetics of molybdocene **catalyzed** hydration of nitriles to amides in aq. soln.)
RN 100-48-1 HCAPLUS
CN 4-Pyridinecarbonitrile (9CI) (CA INDEX NAME)

QD410.07



IT 98-92-0P, Nicotinamide
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(kinetics of molybdocene **catalyzed** hydration of nitriles to amides in aq. soln.)
RN 98-92-0 HCAPLUS
CN 3-Pyridinecarboxamide (9CI) (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2003 ACS

Full Text | Citing References

ACCESSION NUMBER: 1996:431422 HCAPLUS

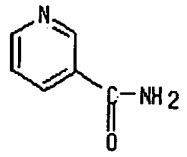
DOCUMENT NUMBER: 125:86507
TITLE: Process and manganese dioxide-based **catalysts** for the preparation of nicotinamide via the hydration of 3-cyanopyridine
INVENTOR(S): Eller, Karsten; Horn, Hans Christoph; Herion, Christof
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 4 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4440927	A1	19960523	DE 1994-4440927	19941117
WO 9616039	A1	19960530	WO 1995-EP4409	19951109
W: AL, AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TT, UA, UG, US, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9538717	A1	19960617	AU 1995-38717	19951109
PRIORITY APPLN. INFO.:			DE 1994-4440927	19941117
			WO 1995-EP4409	19951109

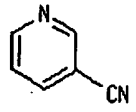
OTHER SOURCE(S): CASREACT 125:86507

AB Nicotinamide is prepd. in high yield and selectivity by the hydration of 3-cyanopyridine in the presence of a mech. stabile **catalyst** comprising: (a) MnO2 30-95; (b) Al2O3 0.5-70, or SiO2, TiO2, or ZrO2 1-70; and (c) alkali **metal** oxides or alk. earth **metal** oxides 0.1-10%.

IT **98-92-0P**, Nicotinamide
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(process and manganese dioxide-based **catalysts** for the prepn. of nicotinamide via the hydration of 3-cyanopyridine)
RN 98-92-0 HCAPLUS
CN 3-Pyridinecarboxamide (9CI) (CA INDEX NAME)



IT **100-54-9**, 3-Cyanopyridine
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(process and manganese dioxide-based **catalysts** for the prepn. of nicotinamide via the hydration of 3-cyanopyridine)
RN 100-54-9 HCAPLUS
CN 3-Pyridinecarbonitrile (9CI) (CA INDEX NAME)



L15 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2003 ACS

Full Text | Citing References

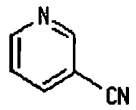
ACCESSION NUMBER: 1992:128194 HCAPLUS
DOCUMENT NUMBER: 116:128194
TITLE: Process for the preparation of copper **catalysts** with increased surface area
INVENTOR(S): Marayti, Ravindranathan; Sivaram, Swaminathan
PATENT ASSIGNEE(S): Indian Petrochemicals Corp. Ltd., India
SOURCE: Indian, 31 pp.
CODEN: INXXAP
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 166044	A	19900303	IN 1986-BO147	19860515
IN 168607	A	19910504	IN 1989-BO63	19890313

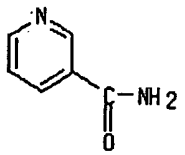
PRIORITY APPLN. INFO.: IN 1986-BO147 19860515
OTHER SOURCE(S): MARPAT 116:128194

AB The title process useful for conversions of partially water-sol. org. nitriles to the corresponding amides, comprises redn. at 0-40° of ≥1 higher valent Cu salts by controlled addn. of an aq. soln. of a reducing agent, such as **metal** borohydride or an aldehyde for 2-5 h. The ratio of Cu salt-reducing agent is 0.5:1.8. After the reaction is complete, the **catalyst** is extd. and washed until the water evinces a pH 5.5-6. CuSO4.5H2O was treated with an alk. soln. of NaBH4 and stirred for 3 h to give the activated **catalyst**. H2C:CHCN was treated with the Cu **catalyst** at a mol. ratio of 2:1, heated to 90° and maintained at this temp. for 2 h with vigorous shaking to give 94.6% H2C:CHCONH2, with a selectivity of 100%.

IT 100-54-9, Nicotinonitrile
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(hydration of, to amide, copper **catalyst** for)
RN 100-54-9 HCAPLUS
CN 3-Pyridinecarbonitrile (9CI) (CA INDEX NAME)



IT 98-92-0P, Nicotinamide
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of, by hydration of nitrile, copper **catalyst** for)
RN 98-92-0 HCAPLUS
CN 3-Pyridinecarboxamide (9CI) (CA INDEX NAME)



L15 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2003 ACS

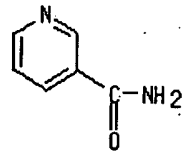
Full Text | Citing References

ACCESSION NUMBER: 1985:476789 HCAPLUS
DOCUMENT NUMBER: 103:76789
TITLE: Study of the activity and selectivity of an supported **catalyst** from oxides of **metals** of varying valence in the oxidative ammonolysis of 3-picoline
AUTHOR(S): Koshevnik, M. A.; German, E. N.; Guseinov, E. M.
CORPORATE SOURCE: USSR
SOURCE: Deposited Doc. (1984), VINITI 5036-84, 123-6 Avail.: VINITI
DOCUMENT TYPE: Report
LANGUAGE: Russian

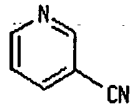
AB The activity and selectivity of the com. **catalyst** KVTS (V and Ti oxides) and of newly prepd. **catalyst** K-3 were studied in oxidative ammonolysis of 3-picoline. The K-3 **catalyst** exhibits high activity and selectivity with 90-93% yield of nicotinic acid amide and nitrile at the total conversion of starting material. It allows 2-3 fold larger productivity of a reactor and decreases energy losses (related with the utilization of large amt. of steam with com. **catalyst**) as compared to the use of KVTS.

IT 98-92-0P 100-54-9P
RL: **RCT (Reactant)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(synthesis of, by oxidative ammonolysis of 3-picoline, activity and reactivity of **catalysts** for)

RN 98-92-0 HCAPLUS
CN 3-Pyridinecarboxamide (9CI) (CA INDEX NAME)



RN 100-54-9 HCAPLUS
CN 3-Pyridinecarbonitrile (9CI) (CA INDEX NAME)



L15 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2003 ACS

Full Text | Citing References

ACCESSION NUMBER: 1974:505297 HCAPLUS
DOCUMENT NUMBER: 81:105297
TITLE: Pyridinecarboxylic acid amides
INVENTOR(S): Watabiki, Yukio; Sugimoto, Nobutaka; Sakai, Koji; Miyoshi, Masamitsu; Uehara, Yoshihiro; Hakozaki, Akiyoshi
PATENT ASSIGNEE(S): Yuki Gosei Kogyo Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

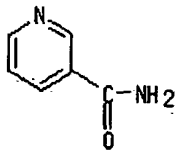
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

JP 49062474	A2	19740617	JP 1972-103976	19721019
JP 51006672	B4	19760301		

PRIORITY APPLN. INFO.: JP 1972-103976 19721019

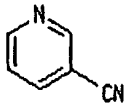
AB Pyridinecarboxylic acid amides were prepd. by hydrolysis of cyanopyridines in the presence of **metal** chromite **catalysts** comprising Cr and Cu (or Zn, Sn, Co, Mn, or Ni). Thus, refluxing a mixt. of 80 g 3-cyanopyridine (I) and 0.5 g Ni chromite **catalyst** in H2O 9 hr gave a product contg. 99.88 mole % (to I) nicotinamide. 4-Cyanopyridine was similarly converted to 98.68 mole % isonicotinamide by use of Cu chromite.

IT 98-92-0P
RL: **PREP (Preparation)**
(from hydrolysis of 3-cyanopyridine)
RN 98-92-0 HCAPLUS
CN 3-Pyridinecarboxamide (9CI) (CA INDEX NAME)



IT 100-48-1
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(hydrolysis of, isonicotinamide from)
RN 100-48-1 HCAPLUS
CN 4-Pyridinecarbonitrile (9CI) (CA INDEX NAME)

IT 100-54-9
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(hydrolysis of, nicotinamide from)
RN 100-54-9 HCAPLUS
CN 3-Pyridinecarbonitrile (9CI) (CA INDEX NAME)



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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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E CYANOPYRIDINE/CN
L2 1 S E3
L3 STRUCTURE UPLOADED
L4 50 S L3
L5 34801 S L3 FULL
L6 STRUCTURE UPLOADED
L7 18 S L6

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L9 5151 S L5/RCT
L10 80 S L9 AND L8

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L11 1 S E3

FILE 'HCAPLUS' ENTERED AT 05:28:39 ON 30 JUN 2003
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L13 0 S L12 AND L10
L14 7 S L10 AND METAL?
L15 5 S L14 AND CATAL?

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There are limits on the size of an answer set being crossed over from one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

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L16 9 L1

=> **s l5**
TOO MANY TERMS FOR FILE CROSSOVER IN L5
There are limits on the size of an answer set being crossed over from

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one file to another.  Enter HELP CROSSOVER at an arrow prompt (=>)
for specific information.

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=> s l1 and l2
                9 L1
                1 L2
L18             0 L1 AND L2

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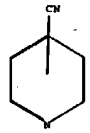

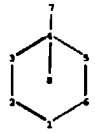

chain nodes :
7
ring nodes :
1 2 3 4 5 6
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS

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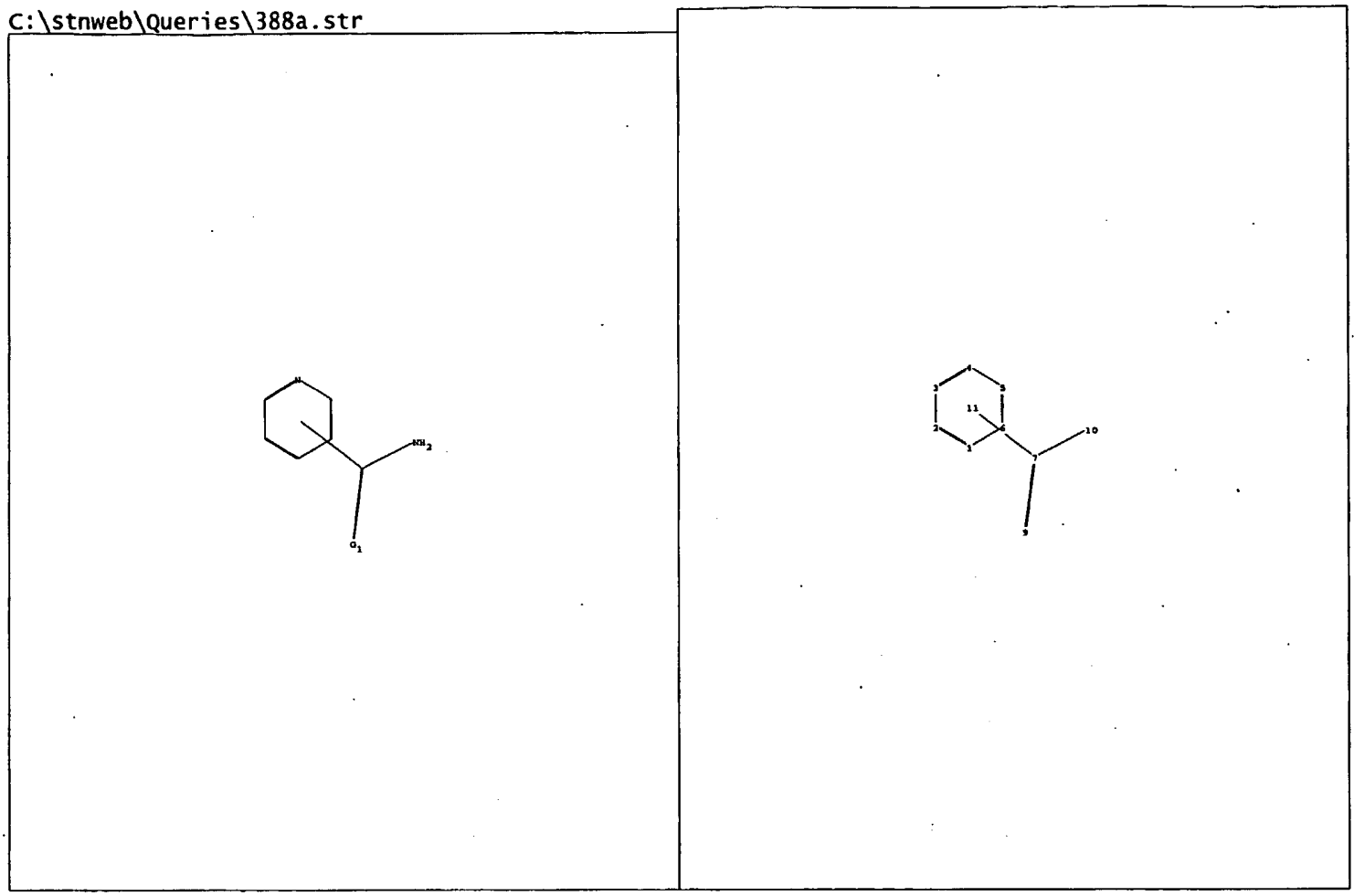

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7 9 10
ring nodes :
1 2 3 4 5 6
chain bonds :
7-9 7-10
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
7-9 7-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS 11:CLASS